

A Markov Basis for Conditional Test of Common Diagonal Effect in Quasi-Independence Model for Square Contingency Tables

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Abstract

In two-way contingency tables we sometimes find that frequencies along the diagonal cells are relatively larger (or smaller) compared to off-diagonal cells, particularly in square tables with the common categories for the rows and the columns. In this case the quasi-independence model with an additional parameter for each of the diagonal cells is usually fitted to the data. A simpler model than the quasi-independence model is to assume a common additional parameter for all the diagonal cells. We consider testing the goodness of fit of the common diagonal effect by Markov chain Monte Carlo (MCMC) method. We derive an explicit form of a Markov basis for performing the conditional test of the common diagonal effect. Once a Markov basis is given, MCMC procedure can be easily implemented by techniques of algebraic statistics. We illustrate the procedure with some real data sets.

1 Introduction

In this paper we discuss a conditional test of a common effect for diagonal cells in two-way contingency tables. Modeling diagonal effects arises mainly in analyzing contingency

tables with common categories for the rows and the columns, although our approach is applicable to general rectangular tables. Many models have been proposed for square contingency tables. Tomizawa [2006] gives a comprehensive review of models for square contingency tables. Gao and Kuriki [2006] discuss testing marginal homogeneity against ordered alternatives.

Goodness of fit tests of these models are usually performed based on the large sample approximation to the null distribution of test statistics. However when a model is expressed in a log-linear form of the cell probabilities, a conditional testing procedure (e.g. the Fisher's exact test for 2×2 contingency tables) can be used. Optimality of conditional tests is a well-known classical fact [Lehmann and Romano, 2005, Chapter 4]. Also large sample approximation may be poor when expected cell frequencies are small (Haberman [1988]).

Sturmfels [1996] and Diaconis and Sturmfels [1998] developed an algebraic algorithm for sampling from conditional distributions for a statistical model of discrete exponential families. This algorithm is applied to conditional tests through the notion of Markov bases. In the Markov chain Monte Carlo approach for testing statistical fitting of the given model, a Markov basis is a set of moves connecting all contingency tables satisfying the given margins. Since then many researchers have extensively studied the structure of Markov bases for models in computational algebraic statistics (e.g. Hoşten and Sullivant [2002], Dobra [2003], Dobra and Sullivant [2004], Geiger et al. [2006], Hara et al. [2007a]).

It has been well-known that for two-way contingency tables with fixed row sums and column sums the set of square-free moves of degree two of the form

$$\begin{array}{cc} +1 & -1 \\ -1 & +1 \end{array}$$

constitutes a Markov basis. However when we impose an additional constraint that the sum of cell frequencies of a subtable S is also fixed, then these moves do not necessarily form a Markov basis. In Hara et al. [2007b] we gave a necessary and sufficient condition on S so that the set of square-free moves of degree two forms a Markov basis. We called this problem a *subtable sum problem*. For the common diagonal effect model defined below in (2) S is the set of diagonal cells. We call this problem a *diagonal sum problem*. By the result of Hara et al. [2007b] we know that the set of square-free moves of degree two does not form a Markov basis for the diagonal sum problem. In this paper we give an explicit form of a Markov basis for the two-way diagonal sum problem. The Markov basis contains moves of degree three and four.

When the sum of cell frequencies of a subtable S is fixed to zero, then the frequency of each cell of S has to be zero and the subtable sum problem reduces to the structural zero case. Contingency tables with structural zero cells are called incomplete contingency tables ([Bishop et al., 1975, Chapter 5]). From the viewpoint of Markov bases, the subtable sum problem is a generalization of the problem concerning structural zeros. Properties of Markov bases for incomplete tables are studied in Aoki and Takemura [2005], Huber et al. [2006], Rapallo [2006].

This paper is organized as follows; In Section 2, we introduce the common diagonal

effect model as a submodel of the quasi-independence model. In Section 3, we summarize some preliminary facts on algebraic statistics and Markov bases. Section 4 shows a Markov basis for contingency tables with fixed row sums, column sums, and the sum of diagonal cells. Numerical examples with some real data sets are given in Section 5. We conclude this paper with some remarks in Section 6.

2 Quasi-Independence model and the common diagonal effect model for two-way contingency tables

Consider an $R \times C$ two-way contingency table $\mathbf{x} = \{x_{ij}\}$, $i = 1, \dots, R$, $j = 1, \dots, C$, where frequencies along the diagonal cells are relatively larger compared to off-diagonal cells. Table 1 [Agresti, 2002, Section 10.5] shows agreement between two pathologists in their diagnoses of carcinoma. We naturally see the tendency that two pathologist agree

Table 1: Diagnoses of carcinoma

	1	2	3	4
1	22	2	2	0
2	5	7	14	0
3	0	2	36	0
4	0	1	17	10

in their diagnoses. Usually the quasi-independence model is fitted to this type of data. In the quasi-independence model, the cell probabilities $\{p_{ij}\}$ are modeled as

$$\log p_{ij} = \mu + \alpha_i + \beta_j + \gamma_i \delta_{ij}, \quad (1)$$

where δ_{ij} is Kronecker's delta. In (1) each diagonal cell (i, i) , $i = 1, \dots, \min(R, C)$, has its own free parameter γ_i . This implies that in the maximum likelihood estimation each diagonal cell is perfectly fitted:

$$\hat{p}_{ii} = \frac{x_{ii}}{n},$$

where $n = \sum_{i=1}^R \sum_{j=1}^C x_{ij}$ is the total frequency.

As a simpler submodel of the quasi-independence model we consider the null hypothesis

$$H : \gamma = \gamma_i, \quad i = 1, \dots, \min(R, C), \quad (2)$$

in the quasi-independence model. We call this model a *common diagonal effect model* and abbreviate it as CDEM hereafter. In CDEM the tendency of the diagonal cells is expressed by a single parameter, rather than perfect fits to diagonal cells. We present some numerical examples of testing CDEM against the quasi-independence model in Section 5.

Both quasi-independence models and CDEM are usually applied to square contingency tables, i.e., $R = C$. As shown in Section 4, however, Markov bases of CDEM does not

essentially depend on the assumption $R = C$. Therefore, in this article, we consider more general cases, i.e., $R \neq C$.

Under CDEM the sufficient statistic consists of the row sums, column sums and the sum of the diagonal frequencies:

$$x_{i+} = \sum_{j=1}^C x_{ij}, \quad i = 1, \dots, R, \quad x_{+j} = \sum_{i=1}^R x_{ij}, \quad j = 1, \dots, C, \quad x_S = \sum_{i=1}^{\min(R,C)} x_{ii}.$$

We write the sufficient statistic as a column vector

$$\mathbf{t} = (x_{1+}, \dots, x_{R+}, x_{+1}, \dots, x_{+C}, x_S)'$$

We also order the elements of \mathbf{x} lexicographically and regard \mathbf{x} as a column vector. Then with an appropriate matrix A_S consisting of 0's and 1's we can write

$$\mathbf{t} = A_S \mathbf{x}.$$

3 Preliminaries on Markov bases

In this section we summarize some preliminary definitions and notations on Markov bases (Diaconis and Sturmfels [1998]). By now Markov bases and their uses are discussed in many papers. See Aoki and Takemura [2005] for example.

The set of contingency tables \mathbf{x} sharing the same sufficient statistic

$$\mathcal{F}_{\mathbf{t}} = \{\mathbf{x} \geq 0 \mid \mathbf{t} = A_S \mathbf{x}\}$$

is called a \mathbf{t} -fiber. An integer table \mathbf{z} is a *move* for A_S if $0 = A_S \mathbf{z}$. By adding a move \mathbf{z} to $\mathbf{x} \in \mathcal{F}_{\mathbf{t}}$, we remain in the same fiber $\mathcal{F}_{\mathbf{t}}$ provided that $\mathbf{x} + \mathbf{z}$ does not contain a negative cell. A finite set of moves $\mathcal{B} = \{\mathbf{z}_1, \dots, \mathbf{z}_L\}$ is a *Markov basis*, if for every \mathbf{t} , $\mathcal{F}_{\mathbf{t}}$ becomes connected by \mathcal{B} , i.e., we can move all over $\mathcal{F}_{\mathbf{t}}$ by adding or subtracting the moves from \mathcal{B} to contingency tables in $\mathcal{F}_{\mathbf{t}}$.

If \mathbf{z} is a move then $-\mathbf{z}$ is a move as well. For convenience we add $-\mathbf{z}$ to \mathcal{B} whenever $\mathbf{z} \in \mathcal{B}$ and only consider sign-invariant Markov bases in this paper. A Markov basis \mathcal{B} is minimal, if every proper sign-invariant subset of \mathcal{B} is no longer a Markov basis. A move \mathbf{z} is called *indispensable* if \mathbf{z} has to belong to every Markov basis. Otherwise \mathbf{z} is called dispensable.

A move \mathbf{z} has positive elements and negative elements. Separating these elements we write $\mathbf{z} = \mathbf{z}^+ - \mathbf{z}^-$, where $(\mathbf{z}^+)_{ij} = \max(\mathbf{z}_{ij}, 0)$ is the positive part and $(\mathbf{z}^-)_{ij} = \max(-\mathbf{z}_{ij}, 0)$ is the negative part of \mathbf{z} . \mathbf{z}^+ and \mathbf{z}^- belong to the same fiber.

We next discuss the notion of distance reduction by a move (Aoki and Takemura [2003], Takemura and Aoki [2005], Hara et al. [2007b]). When $\mathbf{x} + \mathbf{z}$ does not contain a negative cell, we say that \mathbf{z} is applicable to \mathbf{x} . \mathbf{z} is applicable to \mathbf{x} if and only if $\mathbf{z}^- \leq \mathbf{x}$ (inequality for each element). Given two contingency tables \mathbf{x}, \mathbf{y} let $|\mathbf{x} - \mathbf{y}| =$

$\sum_{i,j} |\mathbf{x}_{ij} - \mathbf{y}_{ij}|$ denote the L_1 -distance between \mathbf{x} and \mathbf{y} . For \mathbf{x} and \mathbf{y} in the same fiber, we say that \mathbf{z} reduces their distance if \mathbf{z} or $-\mathbf{z}$ is applicable to \mathbf{x} or \mathbf{y} and the distance $|\mathbf{x} - \mathbf{y}|$ is reduced by the application, e.g. $|\mathbf{x} + \mathbf{z} - \mathbf{y}| < |\mathbf{x} - \mathbf{y}|$. A sufficient condition for \mathbf{z} to reduce the distance between \mathbf{x} and \mathbf{y} is that at least one of the following four conditions hold:

$$\begin{aligned} \text{(i)} \quad & \mathbf{z}^+ \leq \mathbf{x}, \min(\mathbf{z}^-, \mathbf{y}) \neq 0, & \text{(ii)} \quad & \mathbf{z}^+ \leq \mathbf{y}, \min(\mathbf{z}^-, \mathbf{x}) \neq 0, \\ \text{(iii)} \quad & \mathbf{z}^- \leq \mathbf{x}, \min(\mathbf{z}^+, \mathbf{y}) \neq 0, & \text{(iv)} \quad & \mathbf{z}^- \leq \mathbf{y}, \min(\mathbf{z}^+, \mathbf{x}) \neq 0, \end{aligned}$$

where “min” denotes element-wise minimum. We can also think of reducing the distance by a sequence of moves from \mathcal{B} . Clearly a finite set of moves \mathcal{B} is a Markov basis if for every two tables \mathbf{x}, \mathbf{y} from every fiber, we can reduce the distance $|\mathbf{x} - \mathbf{y}|$ by a move \mathbf{z} or a sequence of moves $\mathbf{z}_1, \dots, \mathbf{z}_k$ from \mathcal{B} . We use the argument of distance reduction for proving Theorem 1 in the next section.

We end this section with a known fact for the structural zero problem. In order to state it we introduce two types of moves. In these moves, the non-zero elements are located in the complement S^C of S , i.e., they are in the off-diagonal cells.

- Type I (basic moves in S^C for $\max(R, C) \geq 4$):

$$\begin{array}{cc} & \begin{matrix} j & j' \end{matrix} \\ \begin{matrix} i \\ i' \end{matrix} & \begin{pmatrix} +1 & -1 \\ -1 & +1 \end{pmatrix} \end{array}$$

where i, i', j, j' are all distinct.

- Type II (indispensable moves of degree 3 in S^C for $\min(R, C) \geq 3$):

$$\begin{array}{ccc} & \begin{matrix} i & i' & i'' \end{matrix} \\ \begin{matrix} i \\ i' \\ i'' \end{matrix} & \begin{pmatrix} 0 & +1 & -1 \\ -1 & 0 & +1 \\ +1 & -1 & 0 \end{pmatrix} \end{array}$$

where three zeros are on the diagonal.

Lemma 1. [Aoki and Takemura, 2005, Section 5] *Moves of Type I and II form a minimal Markov basis for the structural zero problem along the diagonal, i.e., $x_{ii} = 0$, $i = 1, \dots, \min(R, C)$.*

4 A Markov basis for the common diagonal effect model

In order to describe a Markov basis for the diagonal sum problem, we introduce four additional types of moves.

- Type III (dispensable moves of degree 3 for $\min(R, C) \geq 3$):

$$\begin{array}{ccccc}
& & i & i' & i'' \\
i & +1 & 0 & -1 & \\
i' & 0 & -1 & +1 & \\
i'' & -1 & +1 & 0 &
\end{array}$$

Note that given three distinct indices i, i', i'' , there are three moves in the same fiber:

$$\begin{array}{ccc}
+1 & 0 & -1 \\
0 & -1 & +1 \\
-1 & +1 & 0
\end{array}
\quad
\begin{array}{ccc}
+1 & -1 & 0 \\
-1 & 0 & +1 \\
0 & +1 & -1
\end{array}
\quad
\begin{array}{ccc}
0 & -1 & +1 \\
-1 & +1 & 0 \\
+1 & 0 & -1
\end{array}$$

Any two of these suffice for the connectivity of the fiber. Therefore we can choose any two moves in this fiber for minimality of Markov basis.

- Type IV (indispensable moves of degree 3 for $\max(R, C) \geq 4$):

$$\begin{array}{ccccc}
& & i & i' & j \\
i & +1 & 0 & -1 & \\
i' & 0 & -1 & +1 & \\
j' & -1 & +1 & 0 &
\end{array}$$

where i, i', j, j' are all distinct. We note that Type IV is similar to Type III but unlike the moves in Type III, the moves of Type IV are indispensable.

- Type V (indispensable moves of degree 4 which are non-square free):

$$\begin{array}{ccccc}
& & j & j' & j'' \\
i & +1 & +1 & -2 & \\
i' & -1 & -1 & +2 &
\end{array}$$

where $i = j$ and $i' = j'$, i.e., two cells are on the diagonal. Note that we also include the transpose of this type as Type V moves.

- Type VI: (square free indispensable moves of degree 4 for $\max(R, C) \geq 4$):

$$\begin{array}{ccccc}
& & j & j' & j'' & j''' \\
i & +1 & +1 & -1 & -1 & \\
i' & -1 & -1 & +1 & +1 &
\end{array}$$

where $i = j$ and $i' = j'$. Type VI includes the transpose of this type.

We now present the main theorem of this paper.

Theorem 1. *The above moves of Types I-VI form a Markov basis for the diagonal sum problem with $\min(R, C) \geq 3$ and $\max(R, C) \geq 4$.*

Proof. Let X, Y be two tables in the same fiber. If

$$x_{ii} = y_{ii}, \quad \forall i = 1, \dots, \min(R, C),$$

then the problem reduces to the structural zero problem and we can use Lemma 1. Therefore we only need to consider the difference

$$X - Y = Z = \{z_{ij}\},$$

where there exists at least one i such that $z_{ii} \neq 0$. Note that in this case there are two indices $i \neq i'$ such that

$$z_{ii} > 0, \quad z_{i'i'} < 0,$$

because the diagonal sum of Z is zero. Without loss of generality we let $i = 1, i' = 2$. We prove the theorem by exhausting various sign patterns of the differences in other cells and confirming the distance reduction by the moves of Types I-VI. We distinguish two cases: $z_{12}z_{21} \geq 0$ and $z_{12}z_{21} < 0$.

Case 1 ($z_{12}z_{21} \geq 0$): In this case without loss of generality assume that $z_{12} \geq 0, z_{21} \geq 0$. Let $0+$ denote the cell with non-negative value of Z and let $*$ denote a cell with arbitrary value of Z . Then Z looks like

$$\begin{array}{cccc} + & 0+ & * & \cdots \\ 0+ & - & * & \cdots \\ * & * & * & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{array}$$

Note that there has to be a negative cell on the first row and on the first column. Let $z_{1j} < 0, z_{j'1} < 0$. Then Z looks like

$$\begin{array}{cccccc} & 1 & 2 & \cdots & j & \cdots \\ 1 & + & 0+ & \cdots & - & \cdots \\ 2 & 0+ & - & \cdots & * & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \cdots \\ j' & - & * & \cdots & * & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

If $j = j'$, we can apply a Type III move to reduce the L_1 distance. If $j \neq j'$, we can apply a Type IV move to reduce the L_1 distance. This takes care of the case $z_{12}z_{21} \geq 0$.

Case 2 ($z_{12}z_{21} < 0$): Without loss of generality assume that $z_{12} > 0, z_{21} < 0$. Then Z looks like

$$\begin{array}{cccc} + & + & * & \cdots \\ - & - & * & \cdots \\ * & * & * & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{array}$$

There has to be a negative cell on the first row and there has to be a positive cell on the second row. Without loss of generality we can let $z_{13} < 0$ and at least one of z_{23}, z_{24} is positive. Therefore Z looks like

$$\begin{array}{cccccc} + & + & - & * & * & \cdots \\ - & - & * & + & * & \cdots \\ * & * & * & * & * & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{array} \quad \text{or} \quad \begin{array}{cccccc} + & + & - & * & \cdots \\ - & - & + & * & \cdots \\ * & * & * & * & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{array} \quad (3)$$

These two cases are not mutually exclusive. We look at Z as the left pattern whenever possible. Namely, whenever we can find two different columns $j, j' \geq 3$, $j \neq j'$ such that $z_{1j}z_{2j'} < 0$, then we consider Z to be of the left pattern. We first take care of the case that Z does not look like the left pattern of (3), i.e., there are no $j, j' \geq 3$, $j \neq j'$, such that $z_{1j}z_{2j'} < 0$.

Case 2-1 (Z does not look like the left pattern of (3)): If there exists some $j \geq 4$ such that $z_{1j} < 0$, then in view of $z_{23} > 0$ we have $z_{1j}z_{23} < 0$ and Z looks like the left pattern of (3). Therefore we can assume

$$z_{1j} \geq 0, \quad \forall j \geq 4.$$

Similarly

$$z_{2j} \leq 0, \quad \forall j \geq 4$$

and Z looks like

$$\begin{array}{cccccc} + & + & - & 0+ & \cdots & 0+ \\ - & - & + & 0- & \cdots & 0- \\ * & * & * & * & \cdots & * \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{array}$$

Because the first row and the second row sum to zero, we have

$$z_{13} \leq -2, \quad z_{23} \geq 2.$$

However then we can apply Type V move to reduce the L_1 distance.

Case 2-2 (Z looks like the left pattern of (3)): Suppose that there exists some $i \geq 3$ such that $z_{i3} > 0$. If $z_{33} > 0$, then Z looks like

$$\begin{array}{cccccc} + & + & - & * & * & \cdots \\ - & - & * & + & * & \cdots \\ * & * & + & * & * & \cdots \\ * & * & * & * & * & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

Then we can apply a type III move involving

$$z_{12} > 0, \quad z_{13} < 0, \quad z_{22} < 0, \quad z_{24} > 0, \quad z_{33} > 0, \quad z_{34} : \text{arbitrary}$$

and reduce the L_1 distance. On the other hand if $z_{i3} > 0$ for $i \geq 4$, then Z looks like

$$\begin{array}{cccccc} + & + & - & * & * & \cdots \\ - & - & * & + & * & \cdots \\ * & * & * & * & * & \cdots \\ * & * & + & * & * & \cdots \\ * & * & * & * & * & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{array}$$

Then we can apply a type IV move involving

$$z_{11} > 0, z_{13} < 0, z_{21} < 0, z_{24} > 0, z_{i3} > 0, z_{ii} : \text{arbitrary}$$

and reduce the L_1 distance. Therefore we only need to consider Z which looks like

$$\begin{array}{cccccc} + & + & - & * & * & \cdots \\ - & - & * & + & * & \cdots \\ * & * & 0- & * & * & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \cdots \\ * & * & 0- & * & * & \cdots \end{array}$$

Similar consideration for the fourth column of Z forces

$$\begin{array}{cccccc} + & + & - & * & * & \cdots \\ - & - & * & + & * & \cdots \\ * & * & 0- & 0+ & * & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \cdots \\ * & * & 0- & 0+ & * & \cdots \end{array}$$

However then because the third column and the fourth column sum to zero, we have $z_{23} > 0$ and $z_{14} < 0$ and Z looks like

$$\begin{array}{cccccc} + & + & - & - & * & \cdots \\ - & - & + & + & * & \cdots \\ * & * & 0- & 0+ & * & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \cdots \\ * & * & 0- & 0+ & * & \cdots \end{array}$$

Then we apply Type VI move to reduce the L_1 distance.

Now we have exhausted all possible sign patterns of Z and shown that the L_1 distance can always be decreased by some move of Types I-VI. \square

Since moves of Type I, II, IV, V and VI are indispensable, we have the following corollary.

Corollary 1. *A minimal Markov basis for the diagonal sum problem with $\min(R, C) \geq 3$ and $\max(R, C) \geq 4$ consists of moves of Types I, II, IV, V, VI and two moves of Type III for each given triple (i, i', i'') .*

5 Numerical examples

In this section with the Markov basis computed in previous sections, we will experiment via MCMC method. Particularly, we test the hypothesis of CDEM for a given data set.

Denote expected cell frequencies under the quasi-independence model and CDEM by

$$\hat{m}_{ij}^{QI} = n\hat{p}_{ij}^{QI}, \quad \hat{m}_{ij}^S = n\hat{p}_{ij}^S,$$

respectively. These expected cell frequencies can be computed via the iterative proportional fitting (IPF). IPF for the quasi-independence model is explained in Chapter 5 of Bishop et al. [1975]. IPF for the common diagonal effect model is given as follows. The superscript k denotes the step count.

1. Set $m_{ij}^{S,k} = m_{ij}^{S,k-1} x_{i+} / m_{i+}^{S,k-1}$ for all i, j and set $k = k + 1$. Then go to Step 2.
2. Set $m_{ij}^{S,k} = m_{ij}^{S,k-1} x_{i+} / m_{i+}^{S,k-1}$ for all i, j and set $k = k + 1$. Then go to Step 3.
3. Set $m_{ii}^{S,k} = m_{ii}^{S,k-1} x_S / m_S^{S,k-1}$ for all $i = 1, \dots, \min(R, C)$ and $m_{ij}^{S,k} = m_{ij}^{S,k-1} (n - m_S^{S,k-1}) / (n - x_S)$ for all $i \neq j$. Then set $k = k + 1$ and go to Step 1.

After convergence we set

$$\hat{m}_{ij}^S = m_{ij}^{S,k} \text{ for all } i, j.$$

We can initialize $m^{S,0}$ by

$$m_{ij}^{S,0} = n / (R \cdot C) \text{ for all } i, j.$$

As the discrepancy measure from the hypothesis of the common diagonal model, we calculate $(2 \times)$ the log likelihood ratio statistic

$$G^2 = 2 \sum_i \sum_j x_{ij} \log \frac{\hat{m}_{ij}^{QI}}{\hat{m}_{ij}^S}.$$

for each sampled table $\mathbf{x} = \{x_{ij}\}$.

In all experiments in this paper, we sampled 10,000 tables after 8,000 burn-in steps.

Example 1. *The first example is from Table 1 of Section 2. The value of G^2 for the observed table in Table 1 is 13.5505 and the corresponding asymptotic p -value is 0.003585 from the asymptotic distribution χ_3^2 .*

A histogram of sampled tables via MCMC with a Markov basis for Table 1 is in Figure 1. We estimated the p -value 0.00379 via MCMC with the Markov basis computed in this paper. Therefore CDEM model is rejected at the significance level of 5%.

Example 2. *The second example is Table 2.12 from Agresti [2002]. Table 2 summarizes responses of 91 married couples in Arizona about how often sex is fun. Columns represent wives' responses and rows represent husbands' responses.*

The value of G^2 for the observed table in Table 2 is 6.18159 and the corresponding asymptotic p -value is 0.1031 from the asymptotic distribution χ_3^2 .

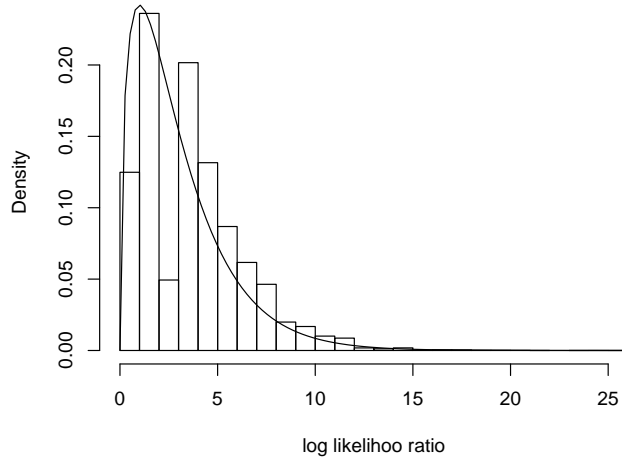


Figure 1: A histogram of sampled tables via MCMC with a Markov basis computed for Table 1. The black line shows the asymptotic distribution χ^2_3 .

Table 2: Married couples in Arizona				
	never/occasionally	fairly often	very often	almost always
never/occasionally	7	7	2	3
fairly often	2	8	3	7
very often	1	5	4	9
almost always	2	8	9	14

A histogram of sampled tables via MCMC with a Markov basis for Table 2 is in Figure 2. We estimated the p -value 0.12403 via MCMC with the Markov basis computed in this paper. Therefore CDEM model is accepted at the significance level of 5%. We also see that χ^2_3 approximates well with this observed data.

Example 3. The third example is Table 1 from Diaconis and Sturmfels [1998]. Table 3 shows data gathered to test the hypothesis of association between birth day and death day. The table records the month of birth and death for 82 descendants of Queen Victoria. A widely stated claim is that birthday-death day pairs are associated. Columns represent the month of birth day and rows represent the month of death day. As discussed in Diaconis and Sturmfels [1998], the Pearson's χ^2 statistic for the usual independence model is 115.6 with 121 degrees of freedom. Therefore the usual independence model is accepted for this data. However, when CDEM is fitted, the Pearson's χ^2 becomes 111.5 with 120 degrees of freedom. Therefore the fit of CDEM is better than the usual independence model.

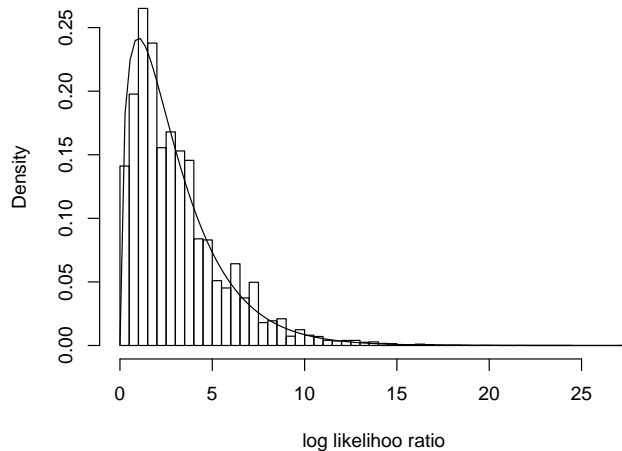


Figure 2: A histogram of sampled tables via MCMC with a Markov basis computed for Table 2. The black line shows the asymptotic distribution χ^2_3 .

Table 3: Relationship between birthday and death day

	Jan	Feb	March	April	May	June	July	Aug	Sep	Oct	Nov	Dec
Jan	1	0	0	0	1	2	0	0	1	0	1	0
Feb	1	0	0	1	0	0	0	0	0	1	0	2
March	1	0	0	0	2	1	0	0	0	0	0	1
April	3	0	2	0	0	0	1	0	1	3	1	1
May	2	1	1	1	1	1	1	1	1	1	1	0
June	2	0	0	0	1	0	0	0	0	0	0	0
July	2	0	2	1	0	0	0	0	1	1	1	2
Aug	0	0	0	3	0	0	1	0	0	1	0	2
Sep	0	0	0	1	1	0	0	0	0	0	1	0
Oct	1	1	0	2	0	0	1	0	0	1	1	0
Nov	0	1	1	1	2	0	0	2	0	1	1	0
Dec	0	1	1	0	0	0	1	0	0	0	0	0

We now test CDEM against the quasi-independence model. The value of G^2 for the observed table in Table 3 is 6.18839 and the corresponding asymptotic p -value is 0.860503 from the asymptotic distribution χ^2_{11} .

A histogram of sampled tables via MCMC with a Markov basis for Table 3 is in Figure 3. We estimated the p -value 0.89454 via MCMC with the Markov basis computed in this paper. There exists a large discrepancy between the asymptotic distribution and the

distribution estimated by MCMC due to the sparsity of the table.

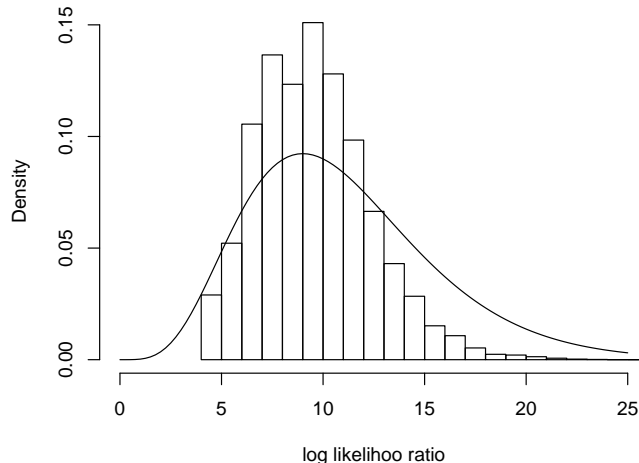


Figure 3: A histogram of sampled tables via MCMC with a Markov basis computed for Table 3. The black line shows the asymptotic distribution χ^2_{11} .

6 Concluding remarks

In this paper we derived an explicit form of a Markov basis for the diagonal sum problem. With this Markov basis we showed that we can easily run the conditional test of the common diagonal effect model. As seen from Figure 3 in Example 3, there may exist a large discrepancy between the asymptotic distribution and the distribution estimated via MCMC. This suggests the efficiency of the conditional test with a Markov basis especially for a sparse table like Table 3.

In Hara et al. [2007b] we gave a necessary and sufficient condition on the subtable S so that the set of square-free moves of degree two forms a Markov basis for S . For a general S it seems to be difficult to explicitly describe a Markov basis. For the diagonal S the Markov basis in Theorem 1 turned out to be relatively simple. It would be helpful to consider some other special type of S in order to understand Markov bases for totally general S .

We have stated Theorem 1 for the case that S contains all the diagonal elements (i, i) , $i = 1, \dots, \min(R, C)$. Actually our proof shows that our result can be generalized to S which is a subset of the diagonal cells. Furthermore we can relabel the rows and the columns. Therefore the essential condition for the result in this paper is that S contains at most one cell in each row and each column of the $R \times C$ table.

Theorem 1 was stated for the case $\min(R, C) \geq 3$ and $\max(R, C) \geq 4$. For smaller tables, we just omit moves, which can not fit into small tables. For completeness we list these cases and give a Markov basis for each case. For avoiding triviality, we assume $\min(R, C) \geq 2$.

1. 2×2 : CDEM is the same as the saturated model and no degrees of freedom is left for the moves
2. 2×3 : Type V moves form a Markov basis.
3. $2 \times C$, $C \geq 4$: Moves of Type I, V and VI form a Markov basis.
4. 3×3 : Moves of Type II, III and V form a Markov basis.

It may be interesting and important to extend the subtable sum or/and diagonal sum problems to higher dimensional tables. However this seems to be difficult at this point and is left for our future studies.

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